Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:23 AM GMT

PDB ID	:	3I9Y
Title	:	Crystal structure of the V. parahaemolyticus histidine kinase sensor TorS sensor domain
Authors	:	Moore, J.O.; Hendrickson, W.A.
Deposited on	:	2009-07-13
Resolution	:	2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

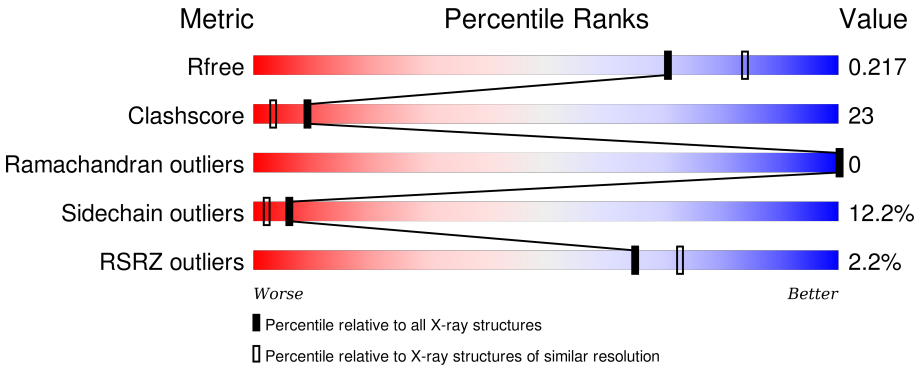
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	2% 37% 31% 12% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1926 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1854	1150	327	370	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	EXPRESSION TAG	UNP Q87ID1
A	48	SER	-	EXPRESSION TAG	UNP Q87ID1
A	49	GLY	-	EXPRESSION TAG	UNP Q87ID1
A	50	SER	-	EXPRESSION TAG	UNP Q87ID1

- Molecule 2 is water.

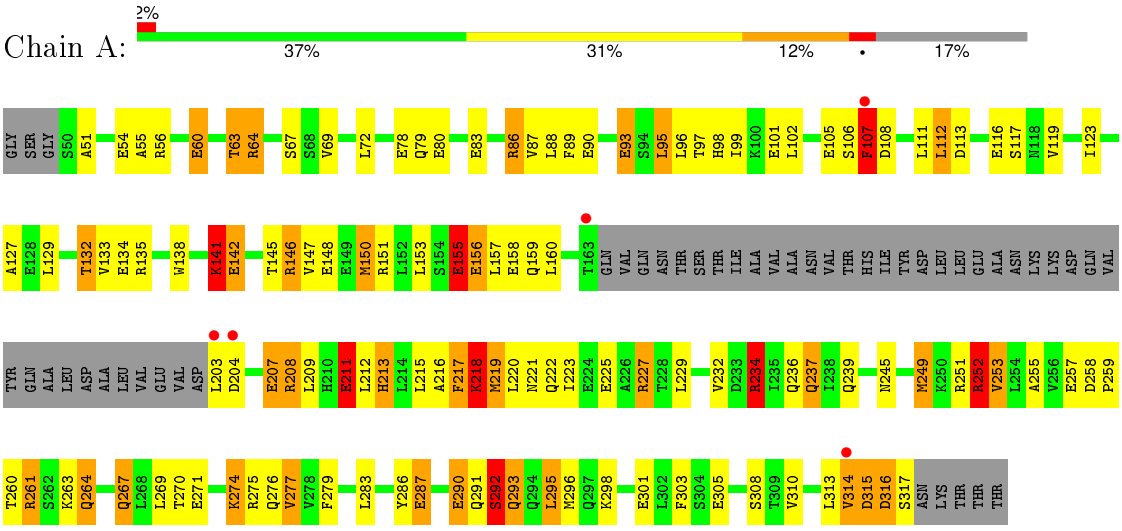
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sensor protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	149.88Å 149.88Å 42.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.16 19.79 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.80-2.16) 99.9 (19.79-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.15Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.261 0.225 , 0.217	Depositor DCC
R_{free} test set	1509 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.0	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29936 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1926	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	2.56	97/1865 (5.2%)	1.95	49/2507 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLU	CD-OE1	16.08	1.43	1.25
1	A	218	LYS	CE-NZ	16.03	1.89	1.49
1	A	211	GLU	CD-OE1	14.97	1.42	1.25
1	A	211	GLU	CG-CD	14.67	1.74	1.51
1	A	93	GLU	CG-CD	13.68	1.72	1.51
1	A	60	GLU	CD-OE2	12.63	1.39	1.25
1	A	155	GLU	CD-OE2	12.51	1.39	1.25
1	A	142	GLU	CB-CG	11.41	1.73	1.52
1	A	287	GLU	CG-CD	11.40	1.69	1.51
1	A	87	VAL	CB-CG2	-11.20	1.29	1.52
1	A	305	GLU	CG-CD	10.83	1.68	1.51
1	A	293	GLN	CG-CD	10.72	1.75	1.51
1	A	218	LYS	CG-CD	10.66	1.88	1.52
1	A	207	GLU	CG-CD	9.96	1.66	1.51
1	A	150	MET	SD-CE	-9.64	1.23	1.77
1	A	303	PHE	CE2-CZ	9.52	1.55	1.37
1	A	305	GLU	CD-OE2	9.48	1.36	1.25
1	A	155	GLU	CG-CD	9.37	1.66	1.51
1	A	305	GLU	CD-OE1	9.35	1.35	1.25
1	A	101	GLU	CB-CG	-9.11	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	LYS	CE-NZ	9.10	1.71	1.49
1	A	155	GLU	CB-CG	9.05	1.69	1.52
1	A	64	ARG	CZ-NH2	8.66	1.44	1.33
1	A	142	GLU	CD-OE2	8.66	1.35	1.25
1	A	290	GLU	CB-CG	-8.55	1.35	1.52
1	A	141	LYS	CD-CE	8.33	1.72	1.51
1	A	156	GLU	CB-CG	-8.15	1.36	1.52
1	A	78	GLU	CG-CD	7.89	1.63	1.51
1	A	218	LYS	CD-CE	7.71	1.70	1.51
1	A	134	GLU	CD-OE2	7.52	1.33	1.25
1	A	207	GLU	CD-OE2	7.37	1.33	1.25
1	A	298	LYS	CE-NZ	7.31	1.67	1.49
1	A	148	GLU	CD-OE1	7.27	1.33	1.25
1	A	142	GLU	CD-OE1	7.19	1.33	1.25
1	A	301	GLU	CG-CD	7.17	1.62	1.51
1	A	225	GLU	CD-OE2	7.12	1.33	1.25
1	A	138	TRP	CE3-CZ3	7.09	1.50	1.38
1	A	314	VAL	CB-CG1	-7.02	1.38	1.52
1	A	218	LYS	CB-CG	7.02	1.71	1.52
1	A	257	GLU	CG-CD	6.99	1.62	1.51
1	A	291	GLN	CG-CD	6.79	1.66	1.51
1	A	107	PHE	CB-CG	6.74	1.62	1.51
1	A	211	GLU	CD-OE2	6.69	1.33	1.25
1	A	134	GLU	CG-CD	6.61	1.61	1.51
1	A	291	GLN	CD-OE1	6.60	1.38	1.24
1	A	134	GLU	CD-OE1	6.57	1.32	1.25
1	A	116	GLU	CD-OE2	6.47	1.32	1.25
1	A	147	VAL	CB-CG1	6.44	1.66	1.52
1	A	78	GLU	CD-OE2	6.43	1.32	1.25
1	A	133	VAL	CB-CG2	6.38	1.66	1.52
1	A	89	PHE	CE2-CZ	6.37	1.49	1.37
1	A	63	THR	CB-CG2	-6.36	1.31	1.52
1	A	60	GLU	CD-OE1	6.35	1.32	1.25
1	A	275	ARG	CG-CD	-6.33	1.36	1.51
1	A	138	TRP	CB-CG	-6.30	1.39	1.50
1	A	132	THR	CB-CG2	-6.21	1.31	1.52
1	A	251	ARG	CZ-NH1	6.12	1.41	1.33
1	A	79	GLN	CG-CD	6.11	1.65	1.51
1	A	208	ARG	CZ-NH1	6.06	1.41	1.33
1	A	141	LYS	CE-NZ	6.02	1.64	1.49
1	A	279	PHE	CE1-CZ	5.96	1.48	1.37
1	A	142	GLU	CG-CD	5.93	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	GLU	CD-OE1	5.89	1.32	1.25
1	A	116	GLU	CG-CD	5.83	1.60	1.51
1	A	217	PHE	CE1-CZ	5.82	1.48	1.37
1	A	151	ARG	CG-CD	5.77	1.66	1.51
1	A	135	ARG	CZ-NH1	5.75	1.40	1.33
1	A	60	GLU	CB-CG	5.74	1.63	1.52
1	A	298	LYS	CD-CE	5.72	1.65	1.51
1	A	293	GLN	CD-NE2	5.71	1.47	1.32
1	A	127	ALA	CA-CB	5.62	1.64	1.52
1	A	237	GLN	CB-CG	-5.58	1.37	1.52
1	A	227	ARG	CZ-NH2	5.56	1.40	1.33
1	A	276	GLN	CA-CB	5.49	1.66	1.53
1	A	83	GLU	CB-CG	5.45	1.62	1.52
1	A	245	ASN	CB-CG	-5.44	1.38	1.51
1	A	72	LEU	CG-CD2	5.40	1.71	1.51
1	A	286	TYR	CD2-CE2	5.40	1.47	1.39
1	A	56	ARG	CG-CD	5.40	1.65	1.51
1	A	138	TRP	CD1-NE1	5.38	1.47	1.38
1	A	90	GLU	CD-OE2	5.37	1.31	1.25
1	A	55	ALA	CA-CB	5.34	1.63	1.52
1	A	80	GLU	CD-OE1	5.32	1.31	1.25
1	A	216	ALA	CA-CB	5.32	1.63	1.52
1	A	249	MET	CB-CG	-5.26	1.34	1.51
1	A	217	PHE	CE2-CZ	5.24	1.47	1.37
1	A	267	GLN	CG-CD	5.20	1.63	1.51
1	A	239	GLN	CG-CD	5.17	1.62	1.51
1	A	215	LEU	CG-CD1	5.16	1.71	1.51
1	A	293	GLN	CD-OE1	5.14	1.35	1.24
1	A	234	ARG	CZ-NH1	5.13	1.39	1.33
1	A	287	GLU	CB-CG	-5.12	1.42	1.52
1	A	208	ARG	CZ-NH2	5.08	1.39	1.33
1	A	255	ALA	CA-CB	-5.07	1.41	1.52
1	A	93	GLU	CD-OE2	5.03	1.31	1.25
1	A	89	PHE	CD1-CE1	5.02	1.49	1.39
1	A	64	ARG	C-O	5.01	1.32	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ARG	NE-CZ-NH1	25.76	133.18	120.30
1	A	227	ARG	NE-CZ-NH2	-16.32	112.14	120.30
1	A	151	ARG	NE-CZ-NH2	11.18	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	157	LEU	CB-CG-CD2	-9.98	94.03	111.00
1	A	150	MET	CG-SD-CE	-9.88	84.39	100.20
1	A	218	LYS	CD-CE-NZ	9.66	133.92	111.70
1	A	277	VAL	CG1-CB-CG2	-9.00	96.50	110.90
1	A	315	ASP	CB-CG-OD1	-8.03	111.08	118.30
1	A	227	ARG	NH1-CZ-NH2	-7.99	110.61	119.40
1	A	208	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	60	GLU	OE1-CD-OE2	7.70	132.54	123.30
1	A	317	SER	N-CA-C	-7.62	90.41	111.00
1	A	60	GLU	CG-CD-OE1	-7.61	103.08	118.30
1	A	208	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	295	LEU	CB-CG-CD1	7.46	123.68	111.00
1	A	315	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	95	LEU	CB-CG-CD2	-7.05	99.01	111.00
1	A	64	ARG	NE-CZ-NH1	-7.05	116.77	120.30
1	A	218	LYS	CG-CD-CE	7.00	132.91	111.90
1	A	141	LYS	CB-CG-CD	-6.92	93.62	111.60
1	A	88	LEU	CB-CG-CD2	-6.64	99.71	111.00
1	A	315	ASP	C-N-CA	6.64	138.31	121.70
1	A	208	ARG	CG-CD-NE	-6.62	97.91	111.80
1	A	153	LEU	CB-CG-CD1	-6.42	100.08	111.00
1	A	295	LEU	CA-CB-CG	6.38	129.99	115.30
1	A	67	SER	CA-CB-OG	-6.08	94.78	111.20
1	A	211	GLU	CG-CD-OE2	-5.97	106.36	118.30
1	A	296	MET	CA-CB-CG	-5.91	103.25	113.30
1	A	219	MET	CA-CB-CG	-5.91	103.25	113.30
1	A	208	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	227	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	112	LEU	CB-CG-CD1	-5.64	101.40	111.00
1	A	64	ARG	CA-CB-CG	-5.55	101.19	113.40
1	A	127	ALA	CB-CA-C	-5.54	101.80	110.10
1	A	275	ARG	CA-CB-CG	-5.50	101.31	113.40
1	A	315	ASP	CA-C-N	-5.36	105.40	117.20
1	A	316	ASP	N-CA-C	-5.32	96.63	111.00
1	A	252	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	86	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	275	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	113	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	237	GLN	N-CA-CB	-5.15	101.33	110.60
1	A	101	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	135	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292	SER	CB-CA-C	5.06	119.72	110.10
1	A	51	ALA	N-CA-C	-5.06	97.34	111.00
1	A	212	LEU	CA-CB-CG	-5.04	103.72	115.30
1	A	287	GLU	OE1-CD-OE2	-5.02	117.27	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1854	0	1897	86	0
2	A	72	0	0	0	0
All	All	1926	0	1897	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:CD	1:A:293:GLN:CG	1.75	1.51
1:A:274:LYS:CE	1:A:274:LYS:NZ	1.71	1.50
1:A:218:LYS:CD	1:A:218:LYS:CG	1.88	1.48
1:A:218:LYS:CE	1:A:218:LYS:NZ	1.89	1.34
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.10	1.10
1:A:261:ARG:HB3	1:A:261:ARG:HH11	1.16	1.07
1:A:261:ARG:HH11	1:A:261:ARG:CB	1.70	1.02
1:A:211:GLU:CD	1:A:252:ARG:HD3	1.79	1.01
1:A:218:LYS:O	1:A:218:LYS:HD2	1.64	0.97
1:A:252:ARG:HH11	1:A:252:ARG:CG	1.81	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:CG2	1:A:292:SER:HB2	2.00	0.90
1:A:315:ASP:OD1	1:A:315:ASP:N	2.08	0.85
1:A:219:MET:SD	1:A:249:MET:HE1	2.17	0.84
1:A:229:LEU:HD13	1:A:234:ARG:HB3	1.64	0.80
1:A:219:MET:SD	1:A:249:MET:CE	2.70	0.79
1:A:132:THR:HG21	1:A:292:SER:HB2	1.64	0.78
1:A:218:LYS:HD2	1:A:222:GLN:HG3	1.66	0.77
1:A:211:GLU:OE2	1:A:252:ARG:HD3	1.84	0.76
1:A:252:ARG:NH1	1:A:252:ARG:HG2	1.91	0.75
1:A:142:GLU:O	1:A:146:ARG:HD2	1.87	0.75
1:A:218:LYS:O	1:A:218:LYS:CD	2.34	0.75
1:A:261:ARG:CB	1:A:261:ARG:NH1	2.50	0.72
1:A:211:GLU:OE2	1:A:252:ARG:NE	2.22	0.72
1:A:211:GLU:OE2	1:A:252:ARG:CD	2.39	0.71
1:A:261:ARG:CG	1:A:261:ARG:HH11	2.04	0.70
1:A:252:ARG:CG	1:A:252:ARG:NH1	2.50	0.68
1:A:204:ASP:HB3	1:A:208:ARG:NH1	2.10	0.67
1:A:261:ARG:CG	1:A:261:ARG:NH1	2.59	0.65
1:A:209:LEU:HD21	1:A:261:ARG:HH22	1.62	0.65
1:A:108:ASP:C	1:A:108:ASP:OD1	2.35	0.64
1:A:158:GLU:OE2	1:A:213:HIS:HD2	1.81	0.63
1:A:218:LYS:HD3	1:A:221:ASN:HB2	1.80	0.63
1:A:209:LEU:CD2	1:A:261:ARG:HH22	2.12	0.62
1:A:274:LYS:CG	1:A:274:LYS:NZ	2.62	0.61
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.67	0.60
1:A:261:ARG:HB3	1:A:261:ARG:NH1	2.01	0.59
1:A:249:MET:HG2	1:A:269:LEU:HD21	1.84	0.58
1:A:211:GLU:OE1	1:A:252:ARG:HD3	2.04	0.58
1:A:106:SER:HB3	1:A:112:LEU:HD21	1.85	0.58
1:A:106:SER:OG	1:A:107:PHE:N	2.37	0.57
1:A:69:VAL:HG13	1:A:129:LEU:HD21	1.87	0.57
1:A:150:MET:SD	1:A:223:ILE:HD13	2.46	0.56
1:A:146:ARG:HH12	1:A:277:VAL:CG2	2.19	0.55
1:A:60:GLU:OE2	1:A:64:ARG:HD3	2.07	0.55
1:A:141:LYS:HE3	1:A:141:LYS:HA	1.89	0.54
1:A:158:GLU:HG3	1:A:217:PHE:CE1	2.42	0.54
1:A:146:ARG:HH12	1:A:277:VAL:HG21	1.72	0.54
1:A:93:GLU:O	1:A:97:THR:HG23	2.08	0.53
1:A:146:ARG:NH1	1:A:277:VAL:CG2	2.72	0.53
1:A:204:ASP:HB3	1:A:208:ARG:HH12	1.73	0.52
1:A:69:VAL:HG13	1:A:129:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:HG2	1:A:156:GLU:N	2.24	0.52
1:A:141:LYS:HE3	1:A:141:LYS:O	2.10	0.52
1:A:60:GLU:OE2	1:A:64:ARG:CD	2.58	0.52
1:A:316:ASP:OD1	1:A:316:ASP:C	2.49	0.51
1:A:219:MET:SD	1:A:249:MET:HE2	2.52	0.50
1:A:258:ASP:HB3	1:A:261:ARG:HG3	1.94	0.50
1:A:314:VAL:C	1:A:315:ASP:OD1	2.51	0.49
1:A:274:LYS:CD	1:A:274:LYS:NZ	2.65	0.48
1:A:249:MET:HG2	1:A:269:LEU:CD2	2.44	0.48
1:A:141:LYS:HE2	1:A:145:THR:OG1	2.13	0.48
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.53	0.47
1:A:313:LEU:O	1:A:316:ASP:HB3	2.14	0.47
1:A:283:LEU:O	1:A:287:GLU:HG3	2.14	0.47
1:A:316:ASP:O	1:A:316:ASP:CG	2.53	0.47
1:A:119:VAL:O	1:A:123:ILE:HG13	2.17	0.45
1:A:54:GLU:OE1	1:A:98:HIS:HD2	1.99	0.44
1:A:232:VAL:O	1:A:236:GLN:HG3	2.17	0.44
1:A:86:ARG:HG2	1:A:86:ARG:NH1	2.33	0.44
1:A:271:GLU:HA	1:A:271:GLU:OE1	2.18	0.44
1:A:260:THR:HG23	1:A:264:GLN:NE2	2.33	0.44
1:A:249:MET:O	1:A:253:VAL:HG13	2.17	0.43
1:A:102:LEU:HD21	1:A:310:VAL:HB	2.00	0.43
1:A:211:GLU:CD	1:A:252:ARG:CD	2.68	0.42
1:A:86:ARG:HH11	1:A:86:ARG:HG2	1.85	0.42
1:A:234:ARG:HD2	1:A:234:ARG:HA	1.55	0.42
1:A:234:ARG:HH11	1:A:237:GLN:HE21	1.68	0.42
1:A:99:ILE:HG23	1:A:99:ILE:HD12	1.67	0.41
1:A:99:ILE:HA	1:A:99:ILE:HD13	1.80	0.41
1:A:274:LYS:HG3	1:A:274:LYS:NZ	2.36	0.40
1:A:258:ASP:HA	1:A:259:PRO:HD2	1.80	0.40
1:A:234:ARG:HH11	1:A:237:GLN:NE2	2.19	0.40
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.78	0.40
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.76	0.40
1:A:209:LEU:HA	1:A:209:LEU:HD23	1.91	0.40
1:A:95:LEU:O	1:A:99:ILE:HG12	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	225/276 (82%)	221 (98%)	4 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	213/253 (84%)	187 (88%)	26 (12%)	6 2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	105	GLU
1	A	107	PHE
1	A	117	SER
1	A	141	LYS
1	A	146	ARG
1	A	155	GLU
1	A	159	GLN
1	A	203	LEU
1	A	207	GLU
1	A	211	GLU
1	A	213	HIS
1	A	218	LYS

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	234	ARG
1	A	252	ARG
1	A	253	VAL
1	A	261	ARG
1	A	263	LYS
1	A	264	GLN
1	A	267	GLN
1	A	270	THR
1	A	290	GLU
1	A	292	SER
1	A	295	LEU
1	A	308	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	98	HIS
1	A	120	GLN
1	A	213	HIS
1	A	237	GLN
1	A	264	GLN
1	A	307	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	229/276 (82%)	-0.07	5 (2%) 65 73	14, 28, 58, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	LEU	5.8
1	A	107	PHE	4.5
1	A	163	THR	4.2
1	A	204	ASP	3.7
1	A	314	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.